=> d his

L3

(FILE 'HOME' ENTERED AT 08:21:42 ON 05 AUG 2002)

FILE 'REGISTRY' ENTERED AT 08:21:57 ON 05 AUG 2002

L1 STRUCTURE UPLOADED

L2 1 S L1

STRUCTURE UPLOADED

L4 0 S L3

L5 38 S L3 FUL

FILE 'CAPLUS' ENTERED AT 08:24:02 ON 05 AUG 2002

L6 47 S L5

L7 STRUCTURE UPLOADED

S L7

FILE 'REGISTRY' ENTERED AT 08:33:01 ON 05 AUG 2002 L8 532 S L7 FUL

FILE 'CAPLUS' ENTERED AT 08:33:15 ON 05 AUG 2002

L9 21 S L8 FUL

L10 STRUCTURE UPLOADED

S L10

FILE 'REGISTRY' ENTERED AT 08:35:06 ON 05 AUG 2002

L11 0 S L10

FILE 'CAPLUS' ENTERED AT 08:35:07 ON 05 AUG 2002

L12 0 S L11 S L10

FILE 'REGISTRY' ENTERED AT 08:35:19 ON 05 AUG 2002

L13 0 S L10

FILE 'CAPLUS' ENTERED AT 08:35:20 ON 05 AUG 2002 L14 0 S L13

FILE 'REGISTRY' ENTERED AT 08:35:26 ON 05 AUG 2002

L15 532 S L9

L16 123 SEARCH L10 SSS SUB=L8 FULL

FILE 'CAPLUS' ENTERED AT 08:39;55 ON 05 AUG 2002

15 L16 applicant work

=> d l10

L10 HAS NO ANSWERS

LIO STR Sel Last Vage (more

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

Structure attributes must be viewed using STN Express query preparation.

=> d 17

L7 HAS NO ANSWERS

L7 STR

=> d bib 117

=> d 19 1-2,4-21 bib abs hitstr

2002:360095 CAPLUS

136:344857

ANSWER 1 OF 21 CAPLUS COPYRIGHT 2002 ACS

L9

AN DN

$$\begin{array}{c} \text{CH} \\ \text{CH}_2 \\ \text{NH} \end{array} \begin{array}{c} \text{CH}_2 \\ \text{O} - 2 \end{array}$$

Structure attributes must be viewed using STN Express query preparation.

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
AN
     2002:122935 CAPLUS
     136:184117
DN
     Preparation of triamine derivative melanocortin receptor ligands
TI
IN
     Watson-Straughan, Karen J.; Gahman, Timothy C.; Qi, Ming; Hamashin,
     Christa; MacDonald, James E.; Green, Michael J.; Holme, Kevin R.;
     Griffith, Michael C.
PΑ
     Lion Bioscience A.-G., Germany
     PCT Int. Appl., 169 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                        KIND DATE
                                                APPLICATION NO.
                                                                   DATE
                        ____
                               -----
                                                -----
ΡI
                                                WO 2001-EP8417
     WO 2002012166
                         A2
                               20020214
                                                                   20010720
     WO 2002012166
                         Α3
                               20020418
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
              HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
              RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
              VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
              DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2001072555
                         Α5
                               20020218
                                               AU 2001-72555
                                                                   20010720
PRAI US 2000-632928
                         Α
                               20000804
     WO 2001-EP8417
                         W
                               20010720
     MARPAT 136:184117
OS
```

TI Immobilized and polymer-supported metal chelate complexes for catalytic hydrolysis and decontamination of pesticides and chemical warfare nerve agents

IN Chang, Eddie L.

PA United States Dept. of the Navy, USA

ODEN: XAXXAV SOLUTION OF THE S

DT Patent

LA English

FAN.CNT 1

PΙ

PATENT NO. KIND DATE APPLICATION NO. DATE
US 862418 A0 20011009 US 2001-862418 20010523

AB Polymer-supported immobilized metal chelate complexes are synthesized and used as reagents for the adsorption and catalytic hydrolysis of phosphorus-contg. esters, esp. phosphates, phosphorofluoridates, phosphonates, and phosphorothionates typically encountered as chem. warfare nerve agents and pesticides. These immobilized metal chelate complexes can be in the form of polymers, micelles, liposomes, phospholipids, tubules, and other self-organized assocns. The polymers can be prepd. in the presence of a target compd. so that the active sites can be molecularly imprinted for better selectivity. Such polymers. which are typically functionalized polyurethanes, acrylates, and vinyl polymers contg. ligand groups, can efficiently decontaminate the above phosphorus-contg. esters (e.g., methylparathion and 4-nitrophenyl phosphate) in a practical and cost-effective manner.

IT 415919-10-7DP, complexes with Cu(2+) salts
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)

(hydrolysis catalysts; immobilized and polymer-supported metal chelate complexes for catalytic hydrolysis and decontamination of pesticides and chem. warfare nerve agents)

RN 415919-10-7 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester, polymer with N-(2-aminoethyl)-N'-[(4-ethenylphenyl)methyl]-1,2-ethanediamine (9CI) (CAINDEX NAME)

CM 1

CRN 106673-77-2 CMF C13 H21 N3

$$H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2$$

CM 2

CRN 3290-92-4 CMF C18 H26 O6

IT 415919-06-1P 415919-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of; in prepn. of immobilized and polymer-supported metal chelate complexes for catalytic hydrolysis and decontamination of pesticides and chem. warfare nerve agents)

RN 415919-06-1 CAPLUS

$$\label{eq:ch2} \begin{array}{c} \text{CH---} \text{CH}_2 \\ \\ \text{H}_2 \text{N---} \text{CH}_2 - \text{NH---} \text{CH}_2 - \text{NH---} \text{CH}_2 \\ \end{array}$$

●3 HCl

RN 415919-10-7 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester, polymer with N-(2-aminoethyl)-N'-[(4-ethenylphenyl)methyl]-1,2-ethanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 106673-77-2 CMF C13 H21 N3

$$H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2$$
 $CH=CH_2$

CM 2

CRN 3290-92-4 CMF C18 H26 O6

L9 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 2002:294231 CAPLUS

DN 136:304058

Method for reducing or preventing the establishment, growth or metastasis TI of cancer by administering PAR-1 and optionally PAR-2 antagonists

D'andrea, Michael; Derian, Claudia; Woodrow, Hal Brent TN

PΔ

so U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 603,229. CODEN: USXXCO

DТ Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002045581	A1	20020418	US 2001-865869	20010525
US 6365617	B1	20020402	US 2000-603229	20000626
PRAI US 1999-141555P	P	19990629		
US 2000-603229	A2	20000626		

MARPAT 136:304058 OS

We have discovered a method of modifying the tumor cell microenvironment AB to reduce or prevent the establishment, growth or metastasis of malignant cells comprising administering to a patient having malignant cells a pharmaceutically effective amt. of a PAR-1 inhibitor and optionally a PAR-2 inhibitor to prevent or reduce activation of normal cells within the tumor microenvironment. This method also has the effect in some patients of modulating the immune system to facilitate a more efficient immune response to malignant cells and maybe coupled with cytokine therapy and T-cell therapy to enhance the patient's immune response to the malignant cells.

314751-99-0 314752-00-6 314752-01-7 ΙT 314752-02-8

> RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(method for reducing or preventing the establishment, growth or metastasis of cancer by administering PAR-1 and optionally PAR-2 antagonists)

ŔŊ

314751-99-0 CAPLUS Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-CN 1H-indazol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(2aminoethyl) - N - (phenylmethyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN314752-00-6 CAPLUS

Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-CN1H-indol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(2-aminoethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

314752-01-7 CAPLUS Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-CN1H-indazol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(4-aminobutyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 314752-02-8 CAPLUS

CN Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1H-indol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(4-aminobutyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L9 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2002 ACS
- AN 2002:121203 CAPLUS
- DN 137:6168
- TI A template synthesis of polyamine macrocycles containing the 1,1'-bis(2-phenol) function
- AU Formica, Mauro; Fusi, Vieri; Giorgi, Luca; Micheloni, Mauro; Palma, Pierangela; Pontellini, Roberto
- CS Institute of Chemical Sciences, University of Urbino, Urbino, 61029, Italy
- SO European Journal of Organic Chemistry (2002), (3), 402-404 CODEN: EJOCFK; ISSN: 1434-193X
- PB Wiley-VCH Verlag GmbH
- DT Journal
- LA English

GΙ

- AB The synthesis of two new polyamine macrocycles I and II, each bearing the 1,1'-bis(2-phenol) group as an integral part of the cyclic framework, is reported. The ligands were obtained by template reactions using a cadmium(II) complex of the suitable polyamine condensed with 3,3'-diformyl-1,1'-bis(2-phenol), followed by selective redn. of the two imine bonds and demetallation in acidic medium.
- IT 433217-50-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of polyamine macrocycles via cadmium-template directed cyclocondensation of polyamines and diformylbisphenol with subsequent imine redn. and demetallation)

- RN 433217-50-6 CAPLUS
- CN Phenol, 2,6-bis[[[2-[(2-aminoethyl)amino]ethyl]amino]methyl]-, hexahydrobromide (9CI) (CA INDEX NAME)

PAGE 1-A

●6 HBr

PAGE 1-B

-- CH2-- CH2-- NH2

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 2002:100868 CAPLUS

DN 136:377283

- TI Switching from intramolecular energy transfer to intramolecular electron transfer by the action of pH and Zn2+ coordination
- AU Albelda, M. Teresa; Diaz, Pilar; Garcia-Espana, Enrique; Lima, Joao C.; Lodeiro, Carlos; Seixas de Melo, J.; Jorge Parola, A.; Pina, Fernando; Soriano, Conxa
- CS Facultat de Quimica, Departament de Quimica Inorganica, Universitat de Valencia, Spain
- SO Chemical Physics Letters (2002), 353(1,2), 63-68 CODEN: CHPLBC; ISSN: 0009-2614
- PB Elsevier Science B.V.
- DT Journal
- LA English
- AB Intramol. electron (eT) and energy transfer (ET) have shown to occur in a covalently linked donor-acceptor (CLDA) system consisting of a naphthalene donor covalently linked through a polyamine chain connector to an anthracene acceptor; the connector has been chosen in order to switch ON or OFF the energy flux as a function of its protonation state as well as by coordination to Zn2+. The largest energy transfer efficiency (.eta.=0.61) occurs for the fully protonated form (pH<2), while at pH>9 (eT) from the lone pairs of the nitrogens to the excited fluorophore takes place, leading to complete quenching of the emission. On the other hand at neutral and basic pH values, coordination of Zn2+ prevents the eT quenching allowing the ET process to occur.
- IT 286833-86-1
 - RL: NUU (Other use, unclassified); USES (Uses)
 (switching from intramol. energy transfer to intramol. electron transfer by action of pH and Zn2+ coordination in relation to)
- RN 286833-86-1 CAPLUS
- CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-(1-naphthalenylmethyl)- (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2$

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L9 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2002 ACS
- AN 2002:32028 CAPLUS
- DN 136:231930
- TI Cesium Effect: High Chemoselectivity in Direct N-Alkylation of Amines
- AU Salvatore, Ralph Nicholas; Nagle, Advait S.; Jung, Kyung Woon
- CS Department of Chemistry, University of South Florida, Tampa, FL, 33620-5250, USA
- SO Journal of Organic Chemistry (2002), 67(3), 674-683 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- AB A novel method for the mono-N-alkylation of primary amines, diamines, and polyamines was developed using cesium bases in order to prep. secondary amines efficiently. A cesium base not only promoted alkylation of primary amines but also suppressed overalkylations of the produced secondary amines. Various amines, alkyl bromides, and alkyl sulfonates were examd., and the results demonstrated that this methodol. was highly chemoselective to favor mono-N-alkylation over dialkylation. In particular, use of

either sterically demanding substrates or amino acid derivs. afforded the secondary amines exclusively, offering wide applications in peptidomimetic syntheses.

IT 324047-67-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (monoalkylation of amines in presence of cesium bases)

RN 324047-67-8 CAPLUS

1,2-Ethanediamine, N-(2-aminoethyl)-N'-(3-phenylpropyl)- (9CI) (CA INDEX CN NAME)

 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-(CH_2)_3-Ph$

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.9 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2002 ACS

ΔN 2001:581397 CAPLUS

135:310754 DN

TIPolyamines containing naphthyl groups as pH-regulated molecular machines driven by light

Albelda, M. Teresa; Diaz, Pilar; Garcia-Espana, Enrique; Bernardo, M. AU Alexandra; Pina, Fernando; Seixas de Melo, J.; Soriano, Conxa; Luis, Santiago V.

Departament de Quimica Inorganica, Facultat de Quimica, Universitat de CS Valencia, Burjassot (Valencia), 46100, Spain

SO Chemical Communications (Cambridge, United Kingdom) (2001), (16), 1520-1521 CODEN: CHCOFS; ISSN: 1359-7345

Royal Society of Chemistry

PB DT Journal

LA English

AΒ A series of compds. made up by linking methylnaphthalene fragments at both ends of different polyamine chains have shown to behave as pH-regulated mol. machines driven by light and fluorescence emission studies have proved the formation of an excimer between the two naphthalene units whose appearance, fluorescence intensity and decay times depend on the pH value of the media.

286833-86-1 IT

> RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(light-driven mol. movements and switched on/off by pH in compds. made up by linking methylnaphthalene fragments at both ends of different polyamine chains)

RN 286833-86-1 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-(1-naphthalenylmethyl)- (9CI) INDEX NAME)

H2N-CH2-CH2-NH-CH2-CH2-NH-CH2

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2002 ACS

```
AN
     2001:152677
                  CAPLUS
DN
     134:193443
ΤI
     Preparation of N-(aminopyrimidinyl)heterocycles as NOS inhibitors
IN
     Arnaiz, Damian O.; Baldwin, John J.; Davey, David D.; Devlin, James J.;
     Dolle, Roland Ellwood, III; Erickson, Shawn David; Mcmillan, Kirk;
     Morrissey, Michael M.; Ohlmeyer, Michael H. J.; Pan, Gonghua; Paradkar,
     Vidyadhar Madhav; Parkinson, John; Phillips, Gary B.; Ye, Bin; Zhao,
     Zuchun
PA
     Berlex Laboratories, Inc., USA; Pharmacopeia, Inc.
SO
     PCT Int. Appl., 45 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
                            _____
                                           -----
                      ____
PΙ
     WO 2001014371
                       A1
                            20010301
                                           WO 2000-US23173
                                                             20000824
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     BR 2000014144
                                          BR 2000-14144
                            20020521
                                                             20000824
                       Α
     EP 1206467
                                           EP 2000-959333
                            20020522
                       Α1
                                                             20000824
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     NO 2002000925
                       Α
                            20020416
                                           NO 2002-925
                                                             20020226
PRAI US 1999-383813
                            19990826
                       A1
     WO 2000-US23173
                       W
                            20000824
os
     MARPAT 134:193443
GΙ
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 $R^4 - (CH_2)_{m_N} (CH_2)_{n} - A$

= CH; n and m = independently 1-4; A = CO2R1 or CONR1R2; R1 = independently H, (ar)alkyl, or aryl; R2 = independently H, alkyl, (CH2) nN(R1) 2, (un) substituted heterocyclylalkyl or aralkyl; when m = 2-4, R4 can be OH, NR1R2, NR1COR1, NR1CO2R1, NR1S(O)tR1, or NR1CON(R1)2; when m = 1-4; R4 can also be CN or heterocyclyl; R5 = H, halo, (ar)alkyl, aryl, or haloalkyl; t = 0-2; and stereoisomers thereof] were prepd. as inhibitors of nitric oxide synthase (NOS). For example, II was formed in a 5-step sequence involving (1) coupling N-cyanoethyl glycine Et ester with 4-chloro-6-methyl-2-methylsulfonylpyrimidine, (2) addn. of imidazole to the pyrimidine, (3) deesterification using LiOH, (4) amidation with Et2NH, and (5) reductive addn. of piperonal to the nitrile using Raney nickel and NaBH(OAc)3. I inhibited nitrogen oxide prodn. in RAW 264.7 mouse monocyte cells and demonstrated the ability to treat the arthritis present in male Lewis rats (no specific data available for either assay). As NOS inhibitors, I are useful in the treatment of pathologies ascribed to abnormalities in nitrogen oxide prodn., e.g. multiple sclerosis, rheumatoid arthritis, dilated cardiomyopathy, and congestive heart failure.

IT 327164-46-5P, 2-[(3-Aminopropyl) [2-(1H-imidazol-1-yl)-6methylpyrimidin-4-yl]amino]-N-[2-(1,3-benzodioxol-5-yl)ethyl]acetamide
327164-47-6P, 2-[(3-Aminopropyl) [2-(1H-imidazol-1-yl)-6methylpyrimidin-4-yl]amino]-N-[2-(4-methoxyphenyl)ethyl]acetamide
327164-48-7P 327164-49-8P, 2-[(3-Aminopropyl)[2-(1Himidazol-1-yl)-6-methylpyrimidin-4-yl]amino]-N-[2-(2,3-dihydrobenzofuran-5yl)ethyl]acetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
 (intermediate; prepn. of heterocyclyl pyrimidinamines as nitric oxide
 synthase inhibitors for treatment of arthritis and other diseases
 related to abnormal NO prodn.)

RN 327164-46-5 CAPLUS

CN Acetamide, 2-[(3-aminopropyl)[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]amino]-N-[2-(1,3-benzodioxol-5-yl)ethyl]- (9CI) (CA INDEX NAME)

RN 327164-47-6 CAPLUS

CN Acetamide, 2-[(3-aminopropyl)[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]amino]-N-[2-(4-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 327164-48-7 CAPLUS

CN Acetamide, 2-[(3-aminopropyl) [2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]amino]-N-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)ethyl]- (9CI) (CA INDEX NAME)

RN 327164-49-8 CAPLUS

CN Acetamide, 2-[(3-aminopropyl)[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]amino]-N-[2-(2,3-dihydro-5-benzofuranyl)ethyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 2001:12414 CAPLUS

DN 134:71904

TI Preparation of indole and indazole urea-peptoids as thrombin receptor antagonists

IN McComsey, David F.; Hoekstra, William J.; Maryanoff, Bruce E.; Zhang,
Han-cheng

PA Ortho-McNeil Pharmaceutical, Inc., USA; Cor Therapeutics, Inc.

SO PCT Int. Appl., 44 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

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PATENT NO.
                       KIND DATE
                                              APPLICATION NO. DATE
                       _ _ _ _
                             -----
                                              -----
ΡI
                                             WO 2000-US18021
     WO 2001000576
                        A1
                              20010104
                                                                20000629
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
              ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
             SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 6365617
                        В1
                              20020402
                                             US 2000-603229 20000626
PRAI US 1999-141555P
                        Ρ
                              19990629
     US 2000-603229
                              20000626
                        Α
os
     MARPAT 134:71904
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$$(R^{8}NHCO)_{m} \xrightarrow{R^{6}} (R^{5})_{n} \xrightarrow{N-CON} (CH_{2})_{p} - R^{1}$$

$$(R^{8}NHCO)_{m} \xrightarrow{R^{7}} (CH_{2})_{n} - R^{2} \qquad (CH_{2})_{n} - R^{2} \qquad I$$

$$(CH_{2})_{p} - R^{1}$$

$$(CH_{2})_{p} - R^{1}$$

$$(CH_{2})_{p} - R^{1}$$

$$(CH_{2})_{n} - R^{2} \qquad I$$

AB Indole and indazole urea-peptoid compds. I [R1 = amino, alkylamino, arylamino, heteroalkyl, etc.; R2 = (un)substituted aryl, arylalkyl, cycloalkyl, heteroaryl; R3 = H, alkyl; R4, R5 = H, alkyl, aminoalkyl, aryl, aralkyl, heteroaryl, cycloalkyl, etc.; R6, R7 = H, alkyl, aminoalkyl, aminocycloalkyl, aryl, heteroarylalkyl, etc.; R8 = H, alkyl, aminoalkyl, allyl, cycloalkyl, aryl, heteroaryl, etc.; X = CH, N; n = 0-3; m = 0 or 1; p = 1 or 2] were prepd. as thrombin receptor antagonists for the treatment of diseases assocd. with thrombosis, restenosis, hypertension, heart failure, arrhythmia, inflammation, angina, stroke, atherosclerosis, ischemic conditions, angiogenesis related disorders, cancer, and neurodegenerative disorders. Thus, compd. II, prepd. by a multistep procedure starting from 6-nitroindole (scheme given), showed IC50 = 1.3 and 0.5 M, resp., in the thrombin-induced gel-filtered platelet aggregation and thrombin receptor binding assays.

IT 314751-99-0P 314752-00-6P 314752-01-7P 314752-02-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of indole and indazole urea-peptoids as thrombin receptor antagonists)

RN 314751-99-0 CAPLUS

CN Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1H-indazol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(2-aminoethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 314752-00-6 CAPLUS

CN Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1H-indol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(2-aminoethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 314752-01-7 CAPLUS

CN Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1H-indazol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(4-aminobutyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 314752-02-8 CAPLUS

CN Glycinamide, N-[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1H-indol-6-yl]amino]carbonyl]-3,4-difluoro-L-phenylalanyl-N2-(4-aminobutyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L9 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2002 ACS
- AN 2000:854989 CAPLUS
- DN 134:147152
- TI CsOH-promoted chemoselective mono-N-alkylation of diamines and polyamines
- AU Salvatore, R. N.; Schmidt, S. E.; Shin, S. I.; Nagle, A. S.; Worrell, J. H.; Jung, K. W.
- CS Department of Chemistry, University of South Florida, Tampa, FL, 33620-5250, USA
- SO Tetrahedron Letters (2000), 41(50), 9705-9708 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier Science Ltd.
- DT Journal

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LA English
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- OS CASREACT 134:147152
- AB Selective N-alkylation of diamines and polyamines was carried out using cesium hydroxide, 4 A mol. sieves, and DMF. This protocol was highly chemoselective, favoring mono-N-alkylation over overalkylations.
- IT 324047-67-8P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (chemoselective mono-N-alkylation of diamines and polyamines promoted by cesium hydroxide)
- RN 324047-67-8 CAPLUS
- CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-(CH_2)_3-Ph$

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L9 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2002 ACS
- AN 2000:682523 CAPLUS
- DN 133:334906
- TI Hydrolysis of p-nitrophenyl acetate promoted by Zn(II) complexes of a linear N3O amine phenol liqand
- AU Xie, Yong-Shu; Lin, Rui-Sen; Liu, Qing-Liang
- CS Department of Chemistry, University of Science and Technology of China, Hefei, 230026, Peop. Rep. China
- SO Wuji Huaxue Xuebao (2000), 16(4), 597-602 CODEN: WHUXEO; ISSN: 1001-4861
- PB Wuji Huaxue Xuebao Bianjibu
- DT Journal
- LA Chinese
- Tetradentate linear ligand N-(2-hydroxybenzyl)diethylenetriamine (HL) was AB synthesized and characterized by elemental anal., IR and 1H NMR. By pH potentiometric titrn. at 25.+-.0.1. degree. and I = 0.1 (KNO3), protonation consts. of the ligand and equil. consts. of Zn(II) complexation with the ligand have been detd. Modes of coordination were discussed, and the dissocn. const. for the phenoxyl and water in the complexes were obtained. The kinetics of p-nitrophenyl acetate (NA) hydrolysis catalyzed by the complexes was detd. spectrophotometrically at 25 + 0.1.degree. and I = 0.1(KNO3) in 10% (V/V) CH3CN at pH 7.0.apprx.9.0 (50 mmol L-1 buffers), and the second-rate consts. kc for NA hydrolysis were obtained. exptl. results indicate that the ligand coordinates with Zn (II) yielding five-coordinated complex with three amino groups, one phenoxyl, and an addnl. water coordinated. The pKa values for the phenoxyl and the water are 5.22 and 9.47 resp. Therefore the complexes can yield nucleophile Zn(II)...-OH, and this has good catalytic effect on NA ester hydrolysis with a kc value of 3.2 x 10-2 mol L-1 s-1 at pH 9.0.
- IT 304681-19-4P
 - RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 - (catalytic ligand precursor; hydrolysis of p-nitrophenyl acetate promoted by Zn(II) complexes of N-(2-hydroxybenzyl)diethylenetriamine)
- RN 304681-19-4 CAPLUS
- CN Phenol, 2-[[[2-[(2-aminoethyl)amino]ethyl]amino]methyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

L9 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 2000:456478 CAPLUS

DN 133:144180

TI Naphthylmethyl polyethylenepolyamine fluorescence chemical sensor

AU Mei, Minghua; Wu, Shikang

CS Institute of Photographic Chemistry, The Chinese Academy of Sciences, Beijing, 100101, Peop. Rep. China

SO Wuli Huaxue Xuebao (2000), 16(6), 559-562 CODEN: WHXUEU; ISSN: 1000-6818

PB Beijing Daxue Chubanshe

DT Journal

LA Chinese

AB Naphthylmethyl polyethylenepolyamines were synthesized. Its complexation with zinc salts in different solvents and the type of formation of the complex were studied by fluorescence spectra. Naphthylmethyl polyethylenepolyamine is a good fluorescence chem. sensor for the testing of foreign zinc ion. A 1:2 stoichiometric complex was found in the soln. of compd. 3 with zinc acetate. But a 1:1 complex was formed when it reacted with zinc chloride in soln. An obvious excimer emission could be obsd. in the fluorescence spectrum of compd. 3 with zinc chloride.

IT 286833-86-1

RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)

(evaluation of naphthylmethyl polyethylenepolyamines as fluorescence chem. sensors for zinc)

RN 286833-86-1 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-(1-naphthalenylmethyl)- (9CI) (CA INDEX NAME)

H₂N-CH₂-CH₂-NH-CH₂-CH₂-NH-CH₂

L9 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 1999:415546 CAPLUS

DN 131:229527

TI Chemical resistance of epoxy polymers depending on a structure amino-phenolic hardeners

AU Moshinsky, Leonid; Figovsky, Oleg L.

CS EPOX Ltd., Kiryat Shmona, 11013, Israel

SO Scientific Israel--Technological Advantages (1999), 1(1), 28-34 CODEN: SITAFG

PB Polymate Ltd., Israeli Research Center

DT Journal

LA English

AB Chem. resistance of polymers based on a row of the polyaminoalkyl phenols (PAP) is described in this article. Tech. clean PAP were synthesized using new, two-stage scheme of reamination of Mannich's bases. Properties of the epoxy polymers tested were optimized on Pareto. Action of dild. water soln. of acids and alkali (20-40%), as well as ethanol, toluene, and acetone was studied. Influence of these media on the polymer oil-absorption and some their properties was researched in detail. Statistical method of design expts. and some math. methods of exptl. data processing were used in the work. As a result, it is ascertained that properties of the epoxy polymers depend from a level of oil-absorption and in less measure depend from hardener structure, and kind of solvent.

IT **244020-63-1P**RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (dependence of chem. resistance of epoxy polymers on amino-phenolic

hardener structure)

RN 244020-63-1 CAPLUS

Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-[[[2-[(2-aminoethyl)amino]ethyl]amino]methyl]phenol, (butoxymethyl)oxirane and (chloromethyl)oxirane (9CI) (CA INDEX NAME)

CM 1

CN

CRN 64349-34-4 CMF C11 H19 N3 O

CM 2

CRN 2426-08-6 CMF C7 H14 O2

CM 3

CRN 106-89-8 CMF C3 H5 Cl O

CM 4

CRN 80-05-7 CMF C15 H16 O2

os

GI

MARPAT 131:5266

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ANSWER 14 OF 21 CAPLUS COPYRIGHT 2002 ACS
L9
     1999:325942 CAPLUS
AN
DN
     131:5266
     Preparation of thienopyrimidines and thienopyridines as anticancer agents
ΤI
     Munchhof, Michael John; Sobolov-Jaynes, Susan Beth
IN
     Pfizer Products Inc., USA
PA
     PCT Int. Appl., 91 pp.
so
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                                              APPLICATION NO.
                                                               DATE
                       KIND
                              DATE
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                                              WO 1998-IB1691
                                                                19981022
PΙ
     WO 9924440
                        A1
                              19990520
             AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE,
             KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW,
             MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
              FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
              CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2309690
                        AΑ
                              19990520
                                              CA 1998-2309690
                                                                19981022
                                              AU 1998-94541
                                                                19981022
     AU 9894541
                        Α1
                              19990531
                                              EP 1998-947716
     EP 1028964
                        Α1
                              20000823
                                                                19981022
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,
             SI, LT, LV, FI, RO
     BR 9814018
                        Α
                              20000926
                                              BR 1998-14018
                                                                 19981022
     JP 2001522853
                        T2
                              20011120
                                              JP 2000-520449
                                                                 19981022
     ZA 9810253
                              20000510
                                              ZA 1998-10253
                                                                 19981110
                        Α
     NO 2000002162
                              20000710
                                              NO 2000-2162
                                                                20000427
                        Α
PRAI US 1997-65097P
                        P
                              19971111
     WO 1998-IB1691
                        W
                              19981022
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The title compds. [I and II; X1 = N, CH; R1 = H, alkyl, C(0)alkyl; R2 = (un)substituted C6-10 aryl, 5-13 membered heterocyclic; R11 = H, alkyl, C(0)NR6R9, etc.; R6 = H, alkyl, etc.; R9 = H, alkyl, etc.] and their pharmaceutically acceptable salts, useful for treating hyperproliferative disorders, were prepd. E.g., a multi-step synthesis of I [X1 = N; R1 = indol-5-yl; R2 = H; R11 = Br], was given. Compds. I are effective at

0.2-2.5 g/day for a 70 kg human.

IT 225384-53-2P 225384-62-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of thienopyrimidines and thienopyridines as anticancer agents)

RN 225384-53-2 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[[4-[7-(1H-indol-5-ylamino)thieno[3,2-b]pyridin-2-yl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{H} \\ \text{NH} \\ \text{NH} \\ \text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}_2-\text{NH}_2 \\ \\ \text{N} \\ \end{array}$$

RN 225384-62-3 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[[4-[7-[(2-methyl-1H-indol-5-yl)amino]thieno[3,2-b]pyridin-2-yl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{H} \\ \text{NH} \\ \text{NH} \\ \text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}_2-\text{NH}_2 \\ \\ \text{N} \\ \end{array}$$

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 1999:132298 CAPLUS

DN 130:215027

TI Redox-driven intramolecular anion translocation between transition metal centers

AU Fabbrizzi, Luigi; Gatti, Francesco; Pallavicini, Piersandro; Zambarbieri, Eugenia

CS Dipartimento di Chimica Generale, Universita di Pavia, Pavia, I-27100, Italy

SO Chemistry--A European Journal (1999), 5(2), 682-690 CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

AB In a two-component system contg. two transition metal centers, M1 and M2, an anion X- coordinated to M1 can be translocated to M2, if (i) the latter metal is redox active (through the M2n+/M2(n+1)+ change) and (ii) the

affinity towards X- decreases along the series: M2(n+1) + > M1 > M2n+. these circumstances, when the M1 apprx. M2 system is in its reduced form, X- stays on M1; on oxidn. X- moves to M2. The above-mentioned model was verified with the covalently linked two-component system N'-(2-aminoethyl)-N-1-[2-[4-(1,4,8,11-tetraazacyclotetradecane-1methyl)benzylamino]ethyl]ethane-1,2-diamine (1), in which a tripodal tetraamine subunit (tren) hosts a CuII ion, and a tetraamine macrocyclic subunit (cyclam) encircles a nickel center, which is redox active through the NiII/NiIII couple. Binding tendencies of inorg. anions towards the CuII, NiII and NiIII ions, in an MeCN soln., were studied and compared with those involving the sep. components [CuII(2)]2+ (2 = N-benzyl-N',N''-bis(2-aminoethyl)ethylenediamine) and [NiII,III(3)]2+/3+ (3 = N-(4-tert-butyl)benzyl-1,4,8,11-tetraazacyclotetradecane). In general, affinity towards X- decreases along the series: NiIII>CuII>NiII. Thus, the authors obsd. through spectroelectrochem. techniques that in the reduced form of the two-component system CuII .apprx. NiII, the X- anion (Cl-, NCO-) is located on the CuII center, whereas on NiII-to-NiIII oxidn. it is translocated to the NiIII center. The translocation is quickly reversible and, in the case of the oxidn. resistant chloride anion, can be carried out indefinitely through consecutive oxidn. and redn. processes, in a controlled potential electrolysis expt. The intramol. nature of the redox-driven anion translocation in the CuII .apprx. NiII,III system is discussed and substantiated by considering the pertinent thermodn. functions .DELTA.Ho and .DELTA.So, obtained by temp. dependent voltammetric studies. The intramol. Cl- translocation from CuII to NiIII prevails over any other intermol. process, due a more favorable entropy contribution.

IT 220980-79-0P

CN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction with nickel perchlorate and copper perchlorate)

RN 220980-79-0 CAPLUS

1,2-Ethanediamine, N,N-bis(2-aminoethyl)-N'-[[4-(1,4,8,11-tetraazacyclotetradec-1-ylmethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L9 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2002 ACS
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AN 1998:774127 CAPLUS

DN 130:162500

TI The molecular design of fluorescent sensors for ionic analytes

AU Fabbrizzi, Luigi; Licchelli, Maurizio; Parodi, Luisa; Poggi, Antonio; Taglietti, Angelo

CS Dipartimento di Chimica Generale, Universita di Pavia, Pavia, I-27100, Italy

SO Journal of Fluorescence (1998), 8(3), 263-271 CODEN: JOFLEN; ISSN: 1053-0509

PB Plenum Publishing Corp.

DT Journal; General Review

LA English

A review with 11 refs. Mol. fluorescent sensors can be synthesized by AΒ covalently linking a photoactive fragment (e.g., anthracene) to a receptor subunit displaying affinity toward the envisaged substrate. The electron transfer process is the privileged signal transduction mechanism: redox active substrates (e.g., transition metals) typically release/uptake an electron to/from the proximate photoexcited fluorophore, the recognition being signaled through fluorescence quenching; redox inactive substrates (d0 and d10 metals, H+) deactivate an existing quenching relay (e.g., a tertiary nitrogen atom close to the fluorophore) and their recognition is signaled through fluorescence enhancement. Anionic substrates can be conveniently recognized from the metal-ligand interaction: polyamine receptors contg. the photophys. inactive ZnIIion bind the carboxylate group. In the case of amino acids, NH3+-CH(R)-COO-, selectivity is improved when the receptor platform bears addnl. groups capable to interact specifically with the R substituent. If R is capable of transferring an electron to the nearby photoexcited fluorophore, the recognition is signaled through fluorescence quenching.

IT 174750-18-6

RL: ARU (Analytical role, unclassified); DEV (Device component use); ANST (Analytical study); USES (Uses)

(mol. design of fluorescent sensors for ionic analytes)

RN 174750-18-6 CAPLUS

CN 1,2-Ethanediamine, N,N-bis(2-aminoethyl)-N'-(9-anthracenylmethyl)- (9CI) (CA INDEX NAME)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 1998:716666 CAPLUS

DN 130:81852

TI Solid-Phase Synthesis of Trisubstituted Bicyclic Guanidines via Cyclization of Reduced N-Acylated Dipeptides

AU Ostresh, John M.; Schoner, Christa C.; Hamashin, Vince T.; Nefzi, Adel; Meyer, Jean-Philippe; Houghten, Richard A.

CS Torrey Pines Institute for Molecular Studies, San Diego, CA, 92121, USA

SO Journal of Organic Chemistry (1998), 63(24), 8622-8623 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

GI

$$R^{1}$$
 R^{2}
 R^{3}
 R^{3}
 R^{3}
 R^{3}
 R^{3}
 R^{1}
 R^{2}
 R^{3}
 R^{3}
 R^{3}
 R^{3}
 R^{3}

AB A novel method for the solid-phase synthesis of trisubstituted bicyclic guanidines I (R1 = CH2Ph, Me, CH2CHMe2, Pr; R2 = CH2Ph, Me, Pr; R3 = CH2CH2Ph, Bu, Et) is presented. The initial reaction step involves the exhaustive redn. of resin-bound N-acylated dipeptides R3CONHCHR2CONHCHR1CONHR (R = polymer support) using borane-THF, followed by cyclization of the resulting triamine with thiocarbonyldiimidazole to generate resin-bound trisubstituted bicyclic guanidines. Cleavage from the resin using HF yields the desired trisubstituted bicyclic guanidines in excellent yield and purity. The approaches described enable efficient high-yield and purity syntheses of either polyamines II or bicyclic guanidines. These methods were applied to the synthesis of both individual compds. and combinatorial libraries.

IT 218931-05-6P

> RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of trisubstituted bicyclic quanidine and linear triamine combinatorial libraries via cyclization and redn. of acylated dipeptide libraries)

RN 218931-05-6 CAPLUS

CN 1,2-Propanediamine, N1-[(1S)-1-(aminomethyl)-2-phenylethyl]-3-phenyl-N2-(2phenylethyl) -, (2S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2002 ACS

1997:673844 CAPLUS AN

127:358467 DN

Synthesis, characterization, and luminescence properties of TI anthrylpolyamines: an experiment for an integrated, advanced laboratory course

ΑU

Pfennig, Brian W.; Newirth, Terry L.; Van Arman, Scott A. Department Chemistry, Vassar College, Poughkeepsie, NY, 12604, USA CS

SO Chemical Educator [Electronic Publication] (1997), 2(4), No pp. Given CODEN: CHEDF5; ISSN: 1430-4171

URL: http://journals.springer-ny.com/sam-bin/swilma/lab.875488922.html

PB Springer

DTJournal; (online computer file)

LΑ English

A 10-wk, open-ended expt. for a junior/senior-level integrated lab. course AB is described. The project involves the synthesis and instrumental characterization of two monosubstituted and two disubstituted

anthrylpolyamines of varying lengths, as well as a detailed investigation of their photophys. and photochem. properties in the presence of polyanions of biol. interest. Depending on the nature of the polyanion, emission quenching of the anthracene chromophore occurs by a template-directed excimer formation, or by an energy-transfer process. A correlation between the charge of the protonated anthrylpolyamines and the degree of emission quenching is also investigated. This project is ideally suited for introducing students to different quenching mechanisms within the context of a research-oriented, integrated lab. experience.

IT 198712-74-2P

CN

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis, characterization, and luminescence properties of anthrylpolyamines: expt. for integrated, advanced lab. course)

RN 198712-74-2 CAPLUS

9,10-Anthracenedimethanamine, N,N'-bis[2-[(2-aminoethyl)amino]ethyl]-, hexahydrochloride (9CI) (CA INDEX NAME)

$$H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2$$
 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2$

●6 HCl

L9 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2002 ACS

AN 1997:636187 CAPLUS

DN 127:293640

TI Preparation of peptidyl .alpha.-ketoamide derivatives as inhibitors of thrombosis

IN Abelman, Matthew M.; Pearson, Daniel A.; Vlasuk, George P.; Webb, Thomas R.

PA Corvas International, Inc., USA

SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 37,574. CODEN: USXXAM

DT Patent

LA English

FAN CNT 2

FAN.CNT 2							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	US 5670479	Α	19970923	US 1994-218329	19940325		
	US 5656600	Α	19970812	US 1993-37574	19930325		
	CA 2158989	AA	19940929	CA 1994-2158989	19940325		
PRAI	US 1993-37574		19930325				
os	MARPAT 127:29364	0					
GI							

Peptidyl .alpha.-ketoamide derivs. I [R1 = alkyl, alkenyl, aryl, aralkyl, AB aralkenyl, alkoxy, alkenyloxy, aryloxy, aralkyloxy; R2 = CO2R3, CH2CO2R3, 1-R3- or 2-R3-tetrazol-5-yl, R3NHCO (R3 = H, alkyl, aralkyl) or R4SO2CH2, R4SO2NH, R4O2CNH (R4 = alkyl), X = (CH2)m (m = 1, 2, 3); B and C are certain peptidyl residues], their pharmaceutically acceptable salts, compns., diagnostic compns. and pharmaceutical compns., were prepd. as inhibitors of thrombosis. Thus, I [R1 = Pr2CH, R2 = CO2H, m = 2, B-C = (Gly)5-Asn-Gly-Asp-Phe-Glu-Glu-Ile-Pro-Glu-Tyr-Leu-OH] was prepd. and assayed for inhibition of thrombin catalytic activity (Ki = 0.0019 nM). IT

Ι

197080-83-4

GΙ

RL: RCT (Reactant); RACT (Reactant or reagent) (peptidyl ketoamide derivs. as inhibitors of thrombosis)

RN 197080-83-4 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[(4-nitrophenyl)methyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

L9 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2002 ACS 1997:258105 CAPLUS ΑN DN126:340645 Fluorescent sensor of imidazole and histidine TI Fabbrizzi, Luigi; Francese, Giancarlo; Licchelli, Maurizio; Perotti, ΑU Angelo; Taglietti, Angelo CS Dip. Chim. Gen., Univ. Pavia, Pavia, 27100, Italy so Chemical Communications (Cambridge) (1997), (6), 581-582 CODEN: CHCOFS; ISSN: 1359-7345 PΒ Royal Society of Chemistry DTJournal English LΑ

CH₂NH (CH₂)₂N (CH₂CH₂NH₂)₂

CH₂NH (CH₂)₂N (CH₂CH₂NH₂)₂

- AB The di-Zn(II) complex of an octamine contg. the anthracene subunit (I) binds both the imidazolate anion and the imidazolate moiety of L-histidine and signals the binding through the fluorescence quenching of the fluorophore.
- RN 189817-03-6 CAPLUS
 CN 9,10-Anthracenedimethanamine, N,N'-bis[2-[bis(2-aminoethyl)amino]ethyl](9CI) (CA INDEX NAME)

$$H_2N-CH_2-CH_2$$
 $H_2N-CH_2-CH_2-N-CH_2-CH_2-NH-CH_2$
 $H_2N-CH_2-CH_2$
 $H_2N-CH_2-CH_2$
 $H_2N-CH_2-CH_2-N-CH_2-CH_2-NH-CH_2$

- L9 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2002 ACS
- AN 1996:96195 CAPLUS
- DN 124:248665
- TI Molecular recognition of carboxylate ions based on the metal-ligand interaction and signaled through fluorescence quenching
- AU De Santis, Giancarlo; Fabbrizzi, Luigi; Licchelli, Maurizio; Poggi, Antonio; Taglietti, Angelo
- CS Dipartimento Chimica Generale, Universita Pavia, Pavia, I-27100, Italy
- SO Angew. Chem., Int. Ed. Engl. (1996), 35(2), 202-4 CODEN: ACIEAY; ISSN: 0570-0833
- DT Journal
- LA English

GI

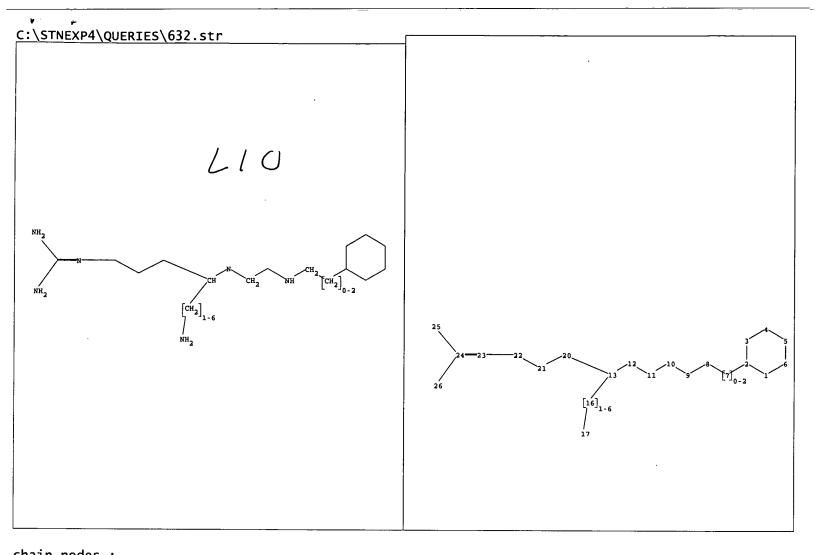
I was prepd. and reacted with Zn(II) to give [ZnI]2+ in which the AB 4-coordinate metal center has a vacant site for the coordination of a solvent mol. or for an anion to give a trigonal-bipyramidal arrangement. When a soln. of [Zni]2+ was titrated with 4-N,N-dimethylaminobenzoate, the fluorescence intensity progressively decreased until completely quenched in contrast to the reaction with BzO- which does not interfere with the photophysics of the proximate anthracene group. Arom. carboxylation ions bearing an acceptor or donor substituent are recognized by the ZnII-contq. receptor 1, and their binding is signaled through quenching of the fluorescence of the appended anthracene unit. Quenching of the fluorophore is induced by an electron transfer to or from the substituent. Fluorescence quenching is not obsd. in the presence of nitrate or thiocyanate but somewhat with chloride indicating the chloride competes with dimethylaminobenzoate for the 5th coordination site. Acetate behaves like chloride. Fluorescence quenching of [ZnI]2+ is also obsd. with 1-ferrocenecarboxylate, 4-nitrobenzoate and 9-anthracenecarboxylate. Partial fluorescence quenching of [CuI]2+ is obsd. even in the absence of any coordinating anion as a result of a direct interaction between the Cu ion and the anthracene group; 4-nitrobenzoate and dimethylaminobenzoate also quench the fluorescence of [CuI]2+.

IT 174750-18-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and complexation with copper and zinc)

RN 174750-18-6 CAPLUS

CN 1,2-Ethanediamine, N,N-bis(2-aminoethyl)-N'-(9-anthracenylmethyl)- (9CI) (CA INDEX NAME)



chain nodes :
 7 8 9 10 11 12 13 16 17 20 21 22 23 24 25 26
ring nodes :
 1 2 3 4 5 6
chain bonds :
 2-7 7-8 8-9 9-10 10-11 11-12 12-13 13-16 13-20 16-17 20-21 21-22 22-23 23-24
 24-25 24-26
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 9-10 12-13 22-23 23-24 24-25 24-26
exact bonds :
 2-7 7-8 8-9 10-11 11-12 13-16 13-20 16-17 20-21 21-22

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS